

# Optimum and quasi-optimum doped superconducting phases in FeAs and Fe<sub>2</sub>As<sub>2</sub> superconductors

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We have developed a real space spin-parallel theory of superconductivity based on the minimum principle in energy. This theory has successfully provided coherent explanations to a number of complicated problems in conventional and non-conventional superconductors. In this paper, we report the study the optimal doping problem in the new oxypnictide high-temperature superconductors using aforementioned theory. In FeAs family, it is shown that there are three optimum (or quasi-optimum) doped phases at doping levels  $x_1 = 1/3, 1/6$  and  $1/8$ , where the vortex lattice forms square or triangular stable configurations. While in Fe<sub>2</sub>As<sub>2</sub> family, the optimal dopings occur at  $x_2 = 2/5$  and  $1/2$  with square and triangular superconducting vortex line lattices, respectively.

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We should not be surprise to find that the iron-based compounds can become superconductors [1, 2, 3, 4]. In fact, superconductivity is a very common physical phenomenon which may occur in any materials with an appropriate charge carrier density (not too high, not too low). It is also not surprising that the pseudogap state (localized Cooper pair) was observed in the underdoped FeAs superconductors [5]. In my opinion, pseudogap is also a common physical phenomenon in some systems where the carrier concentrations are much more sparse and the pair-pair interactions can be neglected [6].

In the face of various superconductors: cuprate, C<sub>60</sub>, MgB<sub>2</sub>, Sr<sub>2</sub>RuO<sub>4</sub>, FeAs, Fe<sub>2</sub>As<sub>2</sub>, etc., it is now clear that we need to develop a unified theory of superconductivity [7]. Without Hamiltonian, without wave function, without electronic bands or orbitals, without quantum field theory, the suggested theory has provided a beautiful and consistent picture for describing the myriad baffling microphenomena which had previously defied explanation. For example, the local checkerboard patterns and “magic doping fractions” in La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> [7], the tetragonal vortex phase in Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8</sub> [8], the hexagonal vortex lattice and charge carrier density in MgB<sub>2</sub> [8], the optimal doping phases [8], pressure effects [9] and pseudogap phase [6] in the new iron-based superconductors, and the  $4a \times 4a$  and  $4\sqrt{2}a \times 4\sqrt{2}a$  checkerboard patterns in hole-doped Ca<sub>2-x</sub>Na<sub>x</sub>CuO<sub>2</sub>Cl<sub>2</sub> [10]. The encouraging agreement of our results with the experiments implies a possibility that our theory would finally open a new window in condensed matter physics.

Although the proposed theory is consistent with many superconducting experimental phenomenology, it is very difficult to persuade people that such a simplistic picture would be the mechanism of Cooper pairing and superconducting in the most complicated strong correlation systems. Obviously, the condensed matter community is unaccustomed to a theory of superconductivity without involving Hamiltonian and wave function. They can't

accept the fact that the Hamiltonian-based famous BCS theory is physically incorrect and even doesn't work for the conventional superconductors [7, 8].

In the present paper, we try to extend the application of the theory to the optimal doping problem in FeAs and Fe<sub>2</sub>As<sub>2</sub> layered superconductors. With this we aim to stress that our theory is based on the most solid *minimum energy principle*, not just arguments or groundless. Physically, in a material, the dominant structural phase should be a minimum-energy state which satisfies the basic symmetry of the crystal structure. In this sense, the superconducting and non-superconducting states are merely some minimum energy condensed states of the electronic charge carriers, or some kinds of real-space low-energy charge orders (the so-called Wigner crystals). In our viewpoint, the minimum-energy based superconducting theory [6, 7, 8, 9, 10] exhibits remarkably the beauty and mystery of physics, moreover, this approach is the most reliable one. Generally, a correct microscopic physical theory should be established in the following way: (the fundamental law of nature: *minimum energy principle*)  $\rightarrow$  (*microscopic symmetry of material structure*)  $\rightarrow$  (*physical or scientific laws*). Here we would like to reemphasize that a correct and reliable physical theory must firstly be mathematically simple and non-approximate. Time can prove that all the existing theories of superconductors based on complex mathematical theorems are indeed on the wrong track.

Fig. 1(a) shows a real-space quasi-zero-dimensional localized Cooper pair. In a previous paper [6], it has been shown that there are two special positions where the localized Cooper pair will be in its minimum energy states. We have argued that pairing in superconductors is an individual behavior characterized by pseudogap, while superconductivity is a collective behavior of many coherent electron pairs [7]. To maintain a stable superconducting phase (minimum energy), first the pairs of electrons must condense themselves into a real-space quasi-

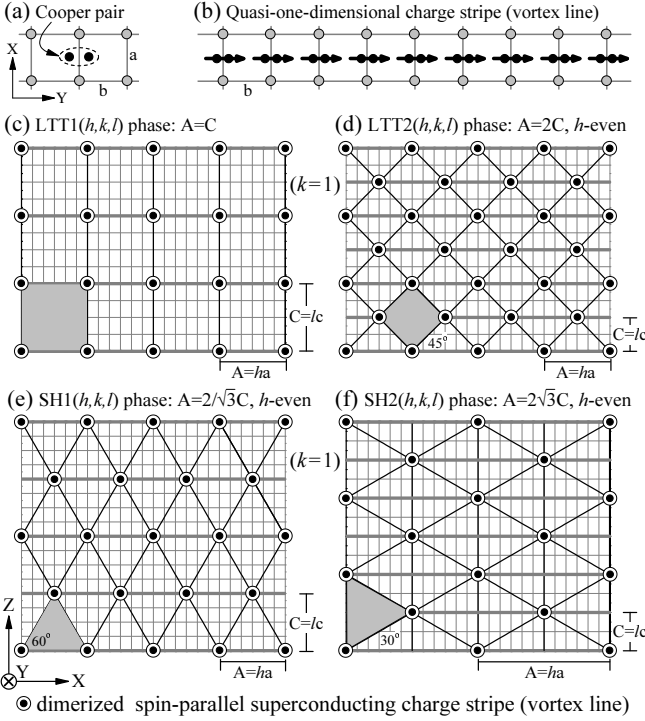


FIG. 1: The schematic interpretation of the theory of superconductivity based on the minimum energy principle in FeAs superconductors. (a) A quasi-zero-dimensional localized Cooper pair, (b) a quasi-one-dimensional dimerized vortex line, (c)-(f) four quasi-two-dimensional vortex lattices with a uniform distribution of vortex lines.

one-dimensional dimerized vortex line (a charge-Peierls dimerized transition), as shown in Fig. 1 (b). Second, the vortex lines can further self-organize into some quasi-two-dimensional vortex lattices where a uniform distribution of vortex lines is formed in the plane perpendicular to the stripes, as shown in Figs. 1 (c)-(f).

In the LTT1( $h, k, l$ ) phase, as shown in Fig. 1(c), the charge stripes have a tetragonal symmetry in XZ plane in which the superlattice constants satisfy

$$\frac{A}{C} = \frac{ha}{lc} = 1. \quad (1)$$

Fig. 1(d) shows the LTT2( $h, k, l$ ), the vortex lattice has a tetragonal symmetry in XZ plane with a orientation  $45^\circ$  and the superlattice constants:

$$\frac{A}{C} = \frac{ha}{lc} = 2. \quad (2)$$

While in simple hexagonal (SH) phases, as shown in Figs. 1(e) and (f), the charge stripes possess identical trigonal crystal structures. In the SH1( $h, k, l$ ) phase [see Fig. 1(e)], the superlattice constants have the following relation

$$\frac{A}{C} = \frac{ha}{lc} = \frac{2\sqrt{3}}{3} \approx 1.15470. \quad (3)$$

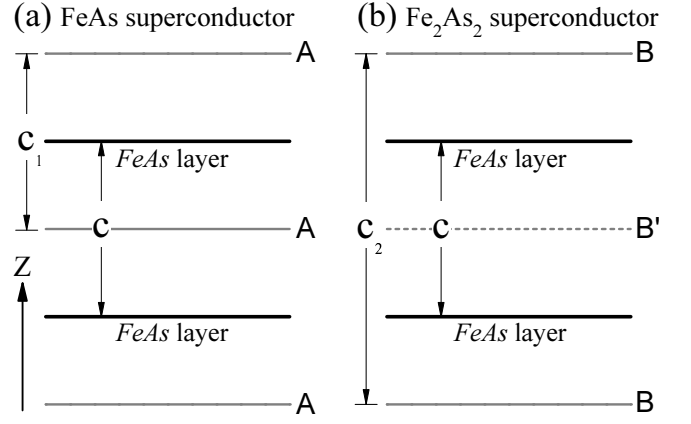


FIG. 2: The schematic plot of the iron-based superconductors. (a) The FeAs compounds, (b) the  $\text{Fe}_2\text{As}_2$  compounds.

For the SH2( $h, k, l$ ) phase of Fig. 1(f), this relation is given by

$$\frac{A}{C} = \frac{ha}{lc} = 2\sqrt{3} \approx 3.46410. \quad (4)$$

The appearance of the stable vortex lattices of Fig. 1 is a common feature of the optimally doped superconducting phases. This in turn leads to some minimum-energy superconducting vortex phases with the highest superconducting transition temperatures of the corresponding superconductors.

After the initial report of  $T_c = 26$  K in  $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$  [1], a new class of FeAs-materials with a promising potential for higher  $T_c$  has been discovered [2]. The structure of these layered compounds is sketched in Fig. 2 (a), where the FeAs layers may contribute to the superconductivity and the A layers are the charge-reservoirs. Figure 2 (b) presents a crystal structure of the new  $\text{Fe}_2\text{As}_2$  family where there are two FeAs superconducting layers within a unit cell of the superconductors, the superconducting currents flow in the FeAs layers, here, the B and B' layers are non-superconducting charge-reservoirs. Some researchers considered that the new iron-based superconductors disclose a new physics, contain new mysteries and may start us along an uncharted pathway to room temperature superconductivity. But we think it is not the appropriate time for us to talk about the room temperature superconductors. What we are more concerned about at present is: which physical parameters play an important role in raising  $T_c$  of the superconductors? According to our theory of Fig. 1,  $T_c$  can be tuned directly by varying the lattice constants and charge carrier density of the superconductors. In other words, for a given superconductor, there exist some optimal matching conditions between the lattice constants and charge carrier density which support the highest superconducting transition temperature of the superconductor, or the optimal doping problem.

TABLE I: Lattice constants, optimal and quasi-optimal superconducting charge-stripe phases (vortex lattices) and doping levels (analytical values  $x = 2/hkl$ ),  $x_1 = x$  and  $x_2 = 2x$  for FeAs and Fe<sub>2</sub>As<sub>2</sub> based superconductors, respectively. Here  $a = a_0\sqrt{2}/2$  is the Fe-Fe distance in two-dimensional square Fe lattices, where  $a_0$  is the lattice constant. The iron layer's distances are  $c = c_1$  and  $c_2/2$  for FeAs and Fe<sub>2</sub>As<sub>2</sub> compounds, respectively. And  $\xi_{xz}$  is the minimum stripe-stripe separation.

Superconductors	$a(\text{\AA})$	$c(\text{\AA})$	$h$	$k$	$l$	$A/C$	$(A/C)_0$	$x$	$x_1 = x$	$x_2 = 2x$	Vortex phase	$\delta(\%)$	$\xi_{xz}(\text{\AA})$
LaO <sub>1-x</sub> F <sub>x</sub> FeAs	2.850	8.739	6	1	1	1.957	2	$1/3 \approx 0.333$	$1/3$		LTT2	2.15	12.360
			6	1	2	0.978	1	$1/6 \approx 0.167$	$1/6$		LTT1	2.15	17.478
			7	1	2	1.141	$2/\sqrt{3}$	$1/7 \approx 0.143$	$1/7$		forbidden	1.19	
			8	1	2	1.304	$2/\sqrt{3}$	$1/8 = 0.125$	$1/8$		SH1	12.7	22.800
SmO <sub>1-x</sub> F <sub>x</sub> FeAs	2.788	8.514	6	1	1	1.965	2	$1/3$	$1/3$		LTT2	1.75	12.041
			6	1	2	0.983	1	$1/6$	$1/6$		LTT1	1.75	16.728
			7	1	2	1.146	$2/\sqrt{3}$	$1/7$	$1/7$		forbidden	0.75	
			8	1	2	1.309	$2/\sqrt{3}$	$1/8$	$1/8$		SH1	13.3	22.304
Cs <sub>1-x</sub> Sr <sub>x</sub> Fe <sub>2</sub> As <sub>2</sub>	2.765	$13.760/2 = 6.880$	5	1	2	1.004	1	$1/5 = 0.20$		0.4	LTT1	0.40	13.825
			8	1	1	3.215	$2\sqrt{3}$	$1/4 = 0.25$		0.5	SH2	7.19	13.760
K <sub>1-x</sub> Sr <sub>x</sub> Fe <sub>2</sub> As <sub>2</sub>	2.751	$12.948/2 = 6.474$	5	1	2	1.062	1	$1/5$		0.4	LTT1	6.20	13.755
			8	1	1	3.399	$2\sqrt{3}$	$1/4$		0.5	SH2	1.78	12.948
Ba <sub>1-x</sub> K <sub>x</sub> Fe <sub>2</sub> As <sub>2</sub>	2.764	$13.212/2 = 6.606$	5	1	2	1.046	1	$1/5$		0.4	LTT1	4.60	13.820
			8	1	1	3.347	$2\sqrt{3}$	$1/4$		0.5	SH2	3.37	13.212

Theoretical and numerical studies have shown that superconductivity in FeAs and Fe<sub>2</sub>As<sub>2</sub> compounds is associated with the two-dimensional square Fe layers. In the framework of the minimum energy of the pairing and superconducting mechanism (see Fig. 1), two types of iron-based superconductors (see Fig. 2) are essentially the same. Based on the experimental data of lattice constants and optimal (or quasi-optimal) vortex phases in the FeAs and Fe<sub>2</sub>As<sub>2</sub> superconductors, as shown in Table I. A new structural parameter  $\delta$  used for evaluating the vortex lattice deformation is given by

$$\delta = \frac{|A/C - (A/C)_0| \times 100}{(A/C)_0} \%,$$

where  $(A/C)_0$  is one of the analytical values of Eqs. (1)-(4) and the  $A/C$  is the corresponding numerical result estimated on the basis of the experimental values of the lattice constants. Normally, the higher the  $\delta$  is, the more serious the vortex lattice deformation, as a consequence, the corresponding superconducting phase may be less stable and exhibit a lower superconducting transition temperature. In addition, a large  $\delta$  value at the same time means a stronger pressure effect on superconductivity in the superconductor.

For the FeAs superconductors, as shown in Table I of LaO<sub>1-x</sub>F<sub>x</sub>FeAs and SmO<sub>1-x</sub>F<sub>x</sub>FeAs, the analytical results indicate that the candidates for the optimal doping vortex phases are LTT2(6,1,1), LTT1(6,1,2) and SH1(8,1,2), respectively. And the corresponding optimal doping levels are  $x_1 = 1/3 \approx 0.333$  [11],  $1/6 \approx 0.167$  [2] and  $1/8 = 0.125$  [1], respectively. These three vortex phases are shown in Fig. 3. From these results, it be-

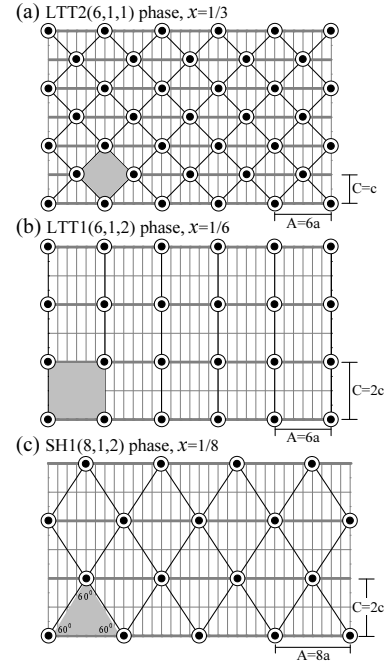


FIG. 3: A schematic description of optimal and quasi-optimal superconducting vortex phases in FeAs superconductor. (a) A crowded quasi-optimal vortex phase at  $x_1 = 1/3$  with a small stripe-stripe separation  $\xi_{xz}$ , (b) the optimal doped phase at  $x_1 = 1/6 = 0.167$ , and (c) a serious distorted quasi-optimal vortex phase at  $x_1 = 0.125$  with a large  $\delta$  value.

comes evident that the LTT1(6,1,2) of Fig. 3 (b) with a small quantity of  $\delta \sim 2\%$  and an appropriate stripe-stripe separation  $\xi_{xz} \sim 17\text{\AA}$  is the optimal doped super-

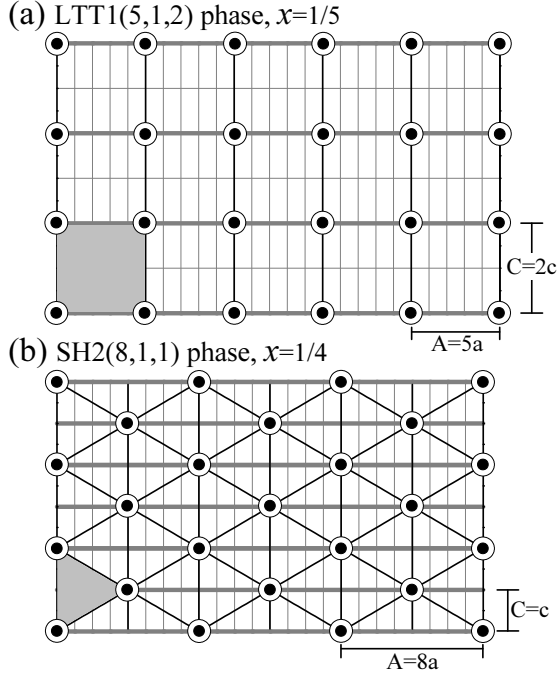


FIG. 4: Two possible optimal doped superconducting vortex lattices in  $\text{Fe}_2\text{As}_2$  superconductors. (a) The square LTT1(5,1,2) at  $x_2 = 2/5 = 0.4$ , and (b) the triangular SH2(8,1,1) at  $x_2 = 1/2 = 0.5$ .

conducting vortex phase, while the LTT2(6,1,1) of Fig. 3 (a) (a crowded vortex lattice with a small  $\xi_{xz} \sim 12\text{\AA}$ ) and SH1(8,1,2) of Fig. 3 (c) (a serious distorted vortex lattice with a large  $\delta \sim 13\%$ ) are the quasi-optimal superconducting phases. The hydrostatic-pressure effects on the superconducting transition temperature of the  $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$  ( $x = 0.11$ ) and  $\text{SmO}_{1-x}\text{F}_x\text{FeAs}$  ( $x = 0.13$ ) sample have been recently reported by three research groups. [12, 13, 14] These results corroborate the suggested external pressure-induced  $T_c$ -enhancement in the compound [9]. It should be pointed out that the three samples lie in the underdoped region with some distorted vortex lattices (for example, SH1(9,1,2) at  $x = 1/9 = 0.11$  and SH1(8,1,2) at  $x = 1/8 = 0.125$ ), in favor of the positive pressure effect on  $T_c$ .

For the  $\text{Fe}_2\text{As}_2$  superconductors [3, 4], there are two competing optimal doped superconducting phases, they are LTT1(5,1,2) of Fig. 4 (a) and SH2(8,1,1) of Fig. 4

(b) with the doping levels  $x_2 = 2/5 = 0.4$  and  $1/2 = 0.5$ , respectively. Experimental results for  $\text{Fe}_2\text{As}_2$  layered compounds show that the optimum doping occurs at  $x_2$  approximately 0.4 [3] or 0.5 [4], which are in good agreement with our analytical results above.

In summary, the optimal doping problem in the new iron-based high-temperature superconductors has been studied by using the newly developed unified theory of superconductivity. In FeAs family, it is shown that the optimum doped phase is LTT1(6,1,2) at doping levels  $x_1 = 1/6$ , where the vortex lattice forms square stable superconducting configuration. Two quasi-optimal doped phases are also analytically determined, they are the square vortex phase of LTT2(6,1,1) at  $x_1 = 1/3$  and the triangular vortex phase of SH1(8,1,2) at  $x_1 = 1/8$ . While in  $\text{Fe}_2\text{As}_2$  family, the theoretical results show that two candidate optimal doping phases are LTT1(5,1,2) at  $x_2 = 2/5$  and SH2(8,1,1) at  $x_2 = 1/2$  with square and triangular superconducting vortex line lattices, respectively.

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